

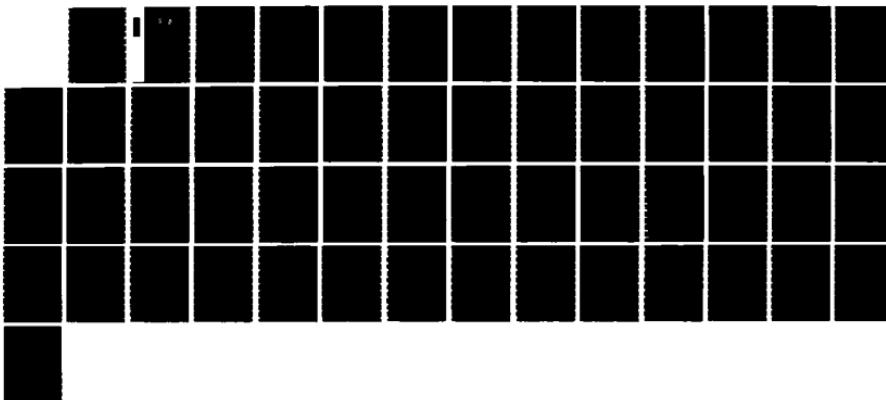
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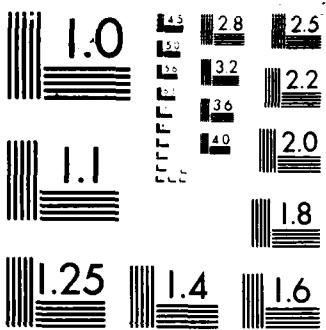
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Technical Report

ON THE CALCULATION OF THE ELECTRON ENERGY SPECTRUM  
IN A WEAKLY IONIZED GAS

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N. J. Carron

MISSION RESEARCH CORPORATION

735 State Street  
Santa Barbara, California 93102

Editor

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Attn: Dr. Robert Barker  
Program Manager

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MISSION RESEARCH CORPORATION  
735 State Street, P. O. Drawer 719  
Santa Barbara, California 93102

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20. ABSTRACT (Continue on reverse if necessary and identify by block number)  We study an approximate solution of the Boltzmann Equation for the distribution of electrons in a weakly ionized gas in the presence of an electric field E, momentum transfer collisions, and inelastic energy transfer collisions. Except when E = 0, we work in the swarm regime where $V_{\text{drift}} \ll V_{\text{thermal}}$ . The mean energy gain rate in the electric field, and mean energy loss rate to collisions are discussed. The importance of spread of energy gain and loss about the mean rates is emphasized, and shown to be critically important in determining the spectrum. A Fokker-Planck (diffusion) type approximation to the collision integral in energy space is developed, leading to a differential equation for the time evolution of the energy spectrum in a time varying field. It should be valid when E varies slowly compared with the mean momentum transfer collision frequency, but on any time scale relative to the energy transfer collision frequency. <i>(continued on next page)</i> <span style="float: right;">cont'd</span>																		
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The steady state spectrum can be obtained in closed form. It reduces to quadratures in terms of the momentum transfer cross section and two sums over energy transfer cross sections. Its connection with ordinary diffusion theory is pointed out. It explains the shortcomings of the Continuous Slowing Down Approximation.

It is demonstrated explicitly for rotational excitations that, when  $E = 0$ , the diffusion approximation reduces to the correct Maxwellian distribution at the gas temperature in the limit that rotational energy spacings become small. The theory is applied to Nitrogen, where energy spectra and transport coefficients are computed, and compared with CSDA calculations, data, and more accurate calculations.



## TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
LIST OF ILLUSTRATIONS	iv
1 INTRODUCTION	1
HISTORICAL	1
APPROXIMATE APPROACH	3
2 THE BOLTZMANN EQUATION	5
LEGENDRE EXPANSION OF THE DISTRIBUTION FUNCTION	6
LEGENDRE EXPANSION OF COLLISION INTEGRAL	7
SLOWLY VARYING FIELDS	8
ENERGY DIFFUSION IN THE ELECTRIC FIELD	9
3 THE INELASTIC COLLISION INTEGRAL	11
MAGNITUDE OF SPREAD IN ENERGY LOSS	13
IMPORTANCE OF ENERGY DIFFUSION	14
CORRECTIONS FOR GAS HEATING	18
4 EQUATION FOR TIME DEPENDENCE OF ENERGY SPECTRUM	19
5 STEADY STATE SPECTRUM	21
THE DRUYVESTEYN SPECTRUM	21
THE NEW TERMS	22
THE LOW ENERGY THERMAL LIMIT	23
6 RELATION TO ORDINARY DIFFUSION THEORY	26
7 THE CASE OF NITROGEN	30
CROSS SECTIONS, AND L AND M FUNCTIONS	30
THE ENERGY SPECTRUM	32
TRANSPORT COEFFICIENTS	35
DISCUSSION	39
APPENDIX A: ROTATIONAL CONTRIBUTION TO L AND M	42
THE SMALL $B_0$ LIMIT	44
REDUCTION OF SPECTRUM TO MAXWELLIAN	46
REFERENCES	47

## LIST OF ILLUSTRATIONS

<u>Figure</u>		<u>Page</u>
1a Balance of mean gain and loss rates.	15	
1b Balance of complete gain and loss rates.	15	
2 Spectrum in N <sub>2</sub> from Equation (36) when E=0.	25	
3a L and M functions for N <sub>2</sub> at 300 K.	31	
3b M/L for N <sub>2</sub> at 300 K.	31	
4 Energy spectrum at E/N <sub>0</sub> = 10 <sup>-16</sup> V-cm <sup>2</sup> from Eq. (36) and in the CSDA.	33	
5 Energy spectrum at 10 <sup>-15</sup> V-cm <sup>2</sup> from Eq. (36), the CSDA, and Reference 18.	34	
6 Calculated N <sub>2</sub> drift velocity (open circles) with data compiled by Dutton (Ref. 8).	36	
7 Calculated swarm characteristic energies in N <sub>2</sub> (open circles) with data compiled by Dutton (Ref. 8).	37	
8 Swarm momentum transfer ( $v_m/N$ ) and energy transfer ( $v_u/N$ ) collision frequencies.	38	
9 Calculated avalanche rates (open circles) with data compiled by Dutton (Ref. 8).	40	

## SECTION 1 INTRODUCTION

The behavior of the electron energy spectrum in a weakly ionized gas in the presence of electric fields, momentum transfer collisions, and energy transfer collisions with the host gas is a long standing problem in plasma physics. Historical surveys appear in References 1 and 2. We have in mind electrons with energy from zero to several eV or a few tens of eV.

The electron energy spectrum controls many processes of interest, such as rates of chemical reactions (attachment, detachment, recombination, etc.), avalanche rate, electrical conductivity and mobility, diffusion, mean electron energy, mean momentum- and energy-transfer collision frequencies, etc. Weakly ionized gases occur frequently in natural and laboratory situations: for example the ambient or nuclear-disturbed ionosphere, and in ionization following dosed air due to gamma-rays (e.g. nuclear EMP), or X-rays, or the passage of fast charged particles. If an electric field is present it can cause the electron cloud to drift, heat it, and possibly produce avalanching.

### HISTORICAL

The spectrum is controlled, of course, by the Boltzmann Equation, and techniques for solving it, and certain progress, were established decades ago (e.g., References 3 and 4). Useful answers were hampered by lack of basic molecular cross sections, and the difficulty of analytically solving the Boltzmann Equation. An expansion in Legendre Polynomials in the angle between the velocity vector and the electric field is useful



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in the swarm regime, in which the drift velocity is small compared with thermal velocity, and this expansion will be employed in the present work, at least in its early stages.

Harder to handle is the collision integral, because of discrete energy loss in inelastic collisions. The integral can be expanded in powers of mean energy loss per collision divided by the average swarm energy. When the expansion is terminated with the first non-trivial term, representing mean energy loss, the ensuing results are called the Continuous Slowing Down Approximation (CSDA). It involves an energy-weighted sum over excitation cross-sections called the "Energy Loss Function", or the "Stopping Cross Section", measuring the mean energy loss rate of mono-energetic electrons.

Data available more recently have made it possible to construct the energy loss function at these relatively low energies where it is extremely difficult to calculate from first principles. (At higher energies,  $> 1$  keV, the Loss Function can be calculated in the Born approximation, where it is known as the Bethe mean stopping power formula.) Using it, energy spectra and bulk plasma parameters computed in the CSDA have been shown to disagree with experimental values by, for example, perhaps 30% for mobilities, and by large factors for the avalanche rate at low temperatures (e.g., Reference 5). Poor agreement with avalanche indicates that the CSDA is particularly deficient in reproducing the high energy tail.

In the special case of constant mean free path and energy loss only to elastic recoil (applicable for example in noble gases at energies below electronic excitation), the transport coefficients computed in the CSDA agree reasonably well with experiments. The spectrum in this case is known as the Druyvesteyn spectrum. Historically it was the first non-Maxwellian spectrum computed for a plasma in the presence of an electric field.

With the advent of better experimental cross-sections and computing facilities attention turned to numerical solutions of the complete Boltzmann Equation with inelastic collision integral, by either Monte Carlo or finite difference techniques. This enabled relatively accurate energy spectra and swarm parameters to be computed, which compare generally quite successfully with experiments. Indeed, one way of determining basic electron-molecule cross-sections is to assume a form for them (guided by previous experiments and quantum-mechanical calculations), and compute the resulting swarm parameters. The cross-sections are then adjusted until computed parameters agree with experimental ones. This technique has been successfully employed by, for example, A. V. Phelps and co-workers over some years (for example, References 6 and 7).

Thus numerical methods exist to compute spectra and transport coefficients. These numerical techniques do not offer physical insight into swarm behavior, and often do not suggest physically-motivated approximation schemes that might be useful in specific applications.

### APPROXIMATE APPROACH

Here we prefer to study more intuitively the processes that determine the spectrum. Our goal is not precise solutions of the Boltzmann Equation. Rather, we build on physically motivated models to construct an approximation to the inelastic collision integral superior to the CSDA. This will lead us to an approximate differential equation for the time evolution of the spectrum in a time varying field, and to a closed form analytic expression for the steady state energy spectrum in terms of the host gas momentum-transfer cross-section and two weighted sums over inelastic energy-transfer cross-sections. The availability of basic electron-molecule cross-sections in interesting gases makes the approach advantageous and useful.

The argument makes clear the importance of spread of energy loss about the mean (energy diffusion, loosely speaking). Usual treatments, such as the CSDA, which retain only the mean energy loss rate, miss a critical piece of the physics determining the spectrum. The approximate spectrum retaining this critical physics can be reduced to quadratures, and is essentially no more complicated in form than the CSDA. It makes clear the physical reason for the inadequacy of the CSDA, and, in particular, it becomes clear why the tail is so low in that approximation. We find the transport coefficients in Nitrogen come out in closer agreement with experiment than in the CSDA. Other gases will be studied in the future. Hopefully the accuracy of the computed coefficients in these gases will be sufficient for a number of applications.

The validity of our approximation (which, as a differential equation, is local in energy space) is still limited by discrete finite energy loss jumps in inelastic processes such as electronic excitations. We require energy steps to be small compared to the spectrum width. Examples of its limitations will be seen in the avalanche rate where our imperfect treatment of energy loss, although improved over the CSDA's, results in a somewhat high rate, and in the  $N_2$  drift velocity at a few eV where the tail of the spectrum can excite electronic states, suddenly decreasing the electron energy by 6 or 7 eV or more. However vibrational excitations cause fractionally small energy transfer, and the approximation appears to be excellent when vibrational excitations dominate, or at higher energies where even electronic levels are not much more energetic than the energy spread in the spectrum itself.

Aside from these problems, the spectrum we deduce reproduces experimental drift velocities and diffusion coefficients very well over some 5 orders of magnitude in the experimental parameter  $E/p$  (the reduced electric field) spanning, for example, essentially the entire range of data compiled by Dutton (Ref. 8).

## SECTION 2 THE BOLTZMANN EQUATION

The Boltzmann Equation for the electron distribution function  $f(\vec{v})$  in an electric field is

$$\frac{\partial f}{\partial t} - \frac{e\vec{E} \cdot \vec{\nabla}_v}{m} f = C + \text{Sources} - \text{Sinks} \quad (1)$$

dropping the spatial gradient term and any magnetic field from the left hand side. Here  $e$  is the magnitude of the electron charge. Sources may be X-ray ionization, or ionization by a fast charged particle. Sinks would include recombination or attachment. Actual sources and sinks are problem specific, and are not considered further here. We concentrate on the effects of the field term and the collision integral  $C$  in determining  $f$ .

Many bulk plasma parameters depend on only the speed distribution function

$$F(v) = \int d\vec{v} f(\vec{v}) \quad (2)$$

or, equivalently, on the energy distribution function  $g(w)$ ,

$$\begin{aligned} g(w) dw &= F(v)v^2 dv, \\ g(w) &= (v/m)F(v) \end{aligned} \quad (3)$$

where  $w = mv^2/2$  is the electron energy. If  $n$  is the number density of particles, the normalizations are

$$n = \int f(\vec{v}) d^3v = \int F(v) v^2 dv = \int g dw \quad (4)$$

The dimensions of  $g$  are, say,  $\text{cm}^{-3} \text{ eV}^{-1}$ . The equilibrium Maxwell distributions for a gas of temperature  $T$  (in energy units), which obtain when  $\vec{E} = 0$ , are

$$\begin{aligned} f_M(\vec{v}) &= n \left( \frac{m}{2\pi T} \right)^{3/2} e^{-mv^2/2T} \\ F_M(v) &= 4\pi f_M \\ g_M(w) &= \frac{2}{\sqrt{\pi}} \frac{n}{T} \left( \frac{w}{T} \right)^{1/2} e^{-w/T} \end{aligned} \quad (5)$$

#### LEGENDRE EXPANSION OF THE DISTRIBUTION FUNCTION

For reduced electric fields not too large, the departure from isotropy will be small, and  $f$  is usefully developed in the usual Legendre Polynomial series in the angle  $\theta$  between  $\vec{v}$  and  $\vec{E}$  (ref. 4)

$$\begin{aligned} f &= \sum_l f_l(v) P_l(\cos\theta) \\ &= f_0 + f_1 \cos\theta + \text{small terms} . \end{aligned} \quad (6)$$

The quantitative criterion is  $V_{\text{drift}} \ll V_{\text{thermal}}$ . When electron-neutral collisions dominate,  $C$  is linear in  $f$ .  $C$  is also expanded, and when the series are inserted in Eq. (1) the  $P_0$  and  $P_1$  parts become

$$\frac{\partial f_0}{\partial t} - \frac{eE}{3m} \cdot 2 \frac{f_1}{v} + \frac{\partial f_1}{\partial v} = C_0 \quad (7a)$$

$$\frac{\partial f_1}{\partial t} - \frac{eE}{m} \frac{\partial f_0}{\partial v} = C_1 \quad (7b)$$

$f_0$  controls the energy spectrum, for  $F$  and  $g$  are

$$F(v) = \int (f_0 + f_1 \cos\theta) d\Omega_v = 4\pi f_0$$
$$\alpha = \frac{4\pi v}{m} f_0 \quad (8)$$

while  $f_1$  controls the bulk electron motion with a drift velocity

$$\vec{v}_d = \frac{1}{n} \int f \vec{v} d^3v = \frac{1}{n} \int (f_0 + f_1 \cos\theta) \vec{v} d^3v$$
$$= \frac{4\pi}{3n} \hat{E} \int f_1 v^3 dv \quad (9)$$

### LEGENDRE EXPANSION OF COLLISION INTEGRAL

Thus  $C_0$  is the contribution of the collision integral to the time rate of change of  $g$ , while  $C_1$  is the contribution of  $C$  to the rate of change of that part of the spectrum that controls the swarm momentum. In general, for a weakly ionized gas in which electron-neutral collisions dominate (ref. 4)

$$C_1 = -v_m f_1 \quad (10)$$

where  $v_m = N_0 v \tau_m$  is the mono-energetic momentum transfer collision frequency,  $\tau_m$  is the momentum transfer cross-section, and  $N_0$  is the background gas number density.

$C_0$  receives contributions from elastic and inelastic processes.

$$C_0 = C_0^{\text{elas}} + C_0^{\text{inelas}} \quad (11)$$

The elastic contributions are from electron energy loss to heavy molecule recoil in an elastic collision, and electron heating by elastic collisions with the host gas at temperature  $T_q$ . These parts are (ref. 4)

$$C_0^{\text{elas}} = \frac{1}{v} \frac{\partial}{\partial(v^2)} \frac{2m}{M_0} v_m v^3 f_0 + \frac{2}{m} \frac{T_q}{\pi} \frac{\partial f_0}{\partial(v^2)} \quad (12)$$

where  $M_0$  is the molecule mass, assumed much greater than the electron mass  $m$ . The first term in Eq. (12) is the mean energy loss rate by elastic collisions. The second term represents the heating rate by the warm gas (the Davydov term). Note the first is essentially proportional to  $\partial f_0 / \partial w$ , while the second is proportional to  $\partial^2 f_0 / \partial w^2$ . The first term is the CSDA to elastic energy loss, and the second is a diffusion-like correction due to gas motion. Higher order corrections (in  $m/M_0$ ) are safely negligible, and the CSDA is adequate for elastic collisions.

$C_0^{\text{inelas}}$  will be treated in the next section.

### SLOWLY VARYING FIELDS

Eq. (10) is inserted into Eq. (7b),

$$\frac{\partial f_1}{\partial t} - \frac{eE}{m} \frac{\partial f_0}{\partial v} = - v_m f_1 \quad (13)$$

When  $a/at \ll v_m$ , we have

$$f_1 = \frac{eE}{mv_m} \frac{\partial f_0}{\partial v} \quad (14)$$

expressing the first order distribution function in terms of the energy spectrum.  $v_m$  is greater than some  $10^{11} \text{ sec}^{-1}$  in sea level air, so condition (14) holds in many circumstances.

To obtain the equation for  $f_0$  we combine the two terms in the first of Eqs. (7) ( $2f_1/v + \partial f_1/\partial v = v^{-2} \partial(v^2 f_1)/\partial v$ ), and insert Eq. (14) for  $f_1$ :

$$\frac{\partial f_0}{\partial t} - \frac{e^2 E^2}{3m^2 v^2} \frac{\partial}{\partial v} \left( \frac{v^2}{v_m} \frac{\partial f_0}{\partial v} \right) = C_0^{\text{elas}} + C_0^{\text{inelas}} \quad (15)$$

We may now transform to an equation for  $g(w)$ :

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial w} \left\{ \frac{e^2 E^2}{m v_m} [g - \frac{2}{3} \frac{\partial}{\partial w} (wg)] \right\} = C_g^{\text{elas}} + C_g^{\text{inelas}} \quad (16)$$

In this equation we have split the electric field term into two parts, one essentially proportional to  $\partial g/\partial w$ , and one to  $\partial^2 g/\partial w^2$ . We also define the collision integral terms on  $g$  rather than  $f_0$ :

$$C_g^{\text{elas}} = \frac{2m}{M_0} \frac{\partial}{\partial w} \left\{ v_m w [g + \sqrt{w} T_g \frac{\partial}{\partial w} (\frac{g}{\sqrt{w}})] \right\} \quad (17)$$

$C_g^{\text{inelas}}$  is taken up in the next section.

### ENERGY DIFFUSION IN THE ELECTRIC FIELD

The two parts of the electric field term in Eq. (16) correspond mathematically to a mean flux ( $\sim \partial g/\partial w$ ) and a diffusive flux ( $\sim \partial^2 g/\partial w^2$ ). That is, elastic scattering in the presence of an electric field produces both a mean gain in energy (rate  $\sim e^2 E^2/m v_m$ ) and a diffusion

in energy (diffusion coefficient  $\sim (2/3)we^2E^2/mv_m$ ). That elastic (or momentum-transfer) scattering causes velocity diffusion is well-known.

That energy diffusion is important can be seen by comparing its effect in Eq. (16) to that of mean energy gain on a Maxwellian distribution of temperature T:

$$\frac{\text{Diffusive Gain}}{\text{Mean Gain}} = \frac{-\frac{2}{3} \frac{\partial}{\partial w} (wg)}{g} = -1 + \frac{2}{3} \frac{w}{T} \quad (18)$$

This is of order unity, and changes sign over the average energy  $3T/2$ . Diffusion allows particles of energy  $w > 3T/2$  to gain energy faster than the mean, and particles with  $w < 3T/2$  to gain energy slower than mean, thus spreading out the spectrum. Diffusion adds body to the spectrum.

### SECTION 3

#### THE INELASTIC COLLISION INTEGRAL

The general form for the collision integral is

$$C_g = \int g(w') P(w', w) dw' - g(w) \int P(w, w') dw' \quad (19)$$

where  $P(w, w') dw'$  is the probability per second that an electron with energy  $w$  collides and ends up with energy  $(w', w'+dw')$ . The CSDA to the elastic part of  $C_g$  was given in Eq(17). For the inelastic part, collisional excitations to discrete molecular states  $k$  of energy  $w_k$  and cross section  $\sigma_k(w)$ , contribute to  $P$  an amount

$$P(w, w') dw' = N_0 v \sum_k \sigma_k \delta(w - w_k - w') dw' \quad (20)$$

assuming all host molecules in the ground state. For a diatomic molecule there will be rotational, vibrational, and electronic states. Excited rotational levels will be populated thermally. This is accounted for in Appendix A in connection with the evaluation of the functions  $L_{in}$  and  $M_{in}$  of Equations (23). For simplicity in the present discussion, we write  $N_0$  as if all molecules were in their ground state. The integrals in Eq. (19) are then readily evaluated for these inelastic processes:

$$C_g^{\text{inelas}} = N_0 \sum_k [(\sigma_k v g)_{w+w_k} - (\sigma_k v g)_w] \quad (21)$$

This clearly exhibits the discrete nature of energy loss,  $g$  being populated at  $w$  by electrons of energy  $w + w_k$ . Since the cross sections  $\sigma_k$  are not exact step functions, the sum  $C_g^{\text{inelas}}$  itself is, of course, a continuous function of  $w$ . Developing the summand in a Taylor Series about  $w$ , we exhibit the first two terms,

$$C_g^{\text{inelas}} = N_0 \frac{\partial}{\partial w} [vgL_{in} + \frac{\partial}{\partial w} (vgM_{in})] + \dots \quad (22)$$

where

$$L_{in} = \sum_k w_k \sigma_k(w) \quad (23a)$$

$$M_{in} = \sum_k \frac{1}{2} w_k^2 \sigma_k(w) \quad (23b)$$

$L_{in}$  is the Energy Loss Function describing the mean energy loss rate to inelastic processes. According to Eq (17), the elastic part of the loss function, for the target molecule at rest, is

$$L_{el} = \frac{2m}{M} \sigma_m w \quad (24)$$

where we have used  $v_m = N_0 v \sigma_m$ . The total mean loss rate to an electron of energy  $w$  is

$$L = L_{el} + L_{in} \quad (25)$$

Since energy loss collisions are probabilistic processes, there will actually be a distribution in the energy loss about the mean rate  $L$ . This is approximated by the  $M_{in}$  term, which can be called the Straggling Function in analogy to the high energy case. This second term in Eq. (22), proportional to  $\partial^2/\partial w^2$ , approximates the true discontinuous random

walk in energy space by a diffusion-like process. Contributions to the Straggling Function from elastic scattering,  $M_{el}$ , are smaller than  $L_{el}$  by  $\sim (m/M_0)w$ , and can be neglected.  $M_{in}$  therefore essentially does not differ from the total Straggling Function  $M = M_{el} + M_{in}$ .

The CSDA neglects the  $M_{in}$  term and retains only the mean loss rate  $L_{in}$  in Eq. (22).

Momentarily neglecting  $T_g$ , Eq. (16) for  $\partial g/\partial t$  now reads

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial w} \left\{ \frac{e^2 E^2}{mv_m} \left[ g - \frac{2}{3} \frac{\partial}{\partial w} (wg) \right] \right\} = N_0 \frac{\partial}{\partial w} [vgL + \frac{\partial}{\partial w} (vgM)] \quad (26)$$

or, in flux conservative form,

$$\frac{\partial g}{\partial t} + \frac{\partial \phi}{\partial w} = 0 \quad (27)$$

where

$$\phi = \frac{e^2 E^2}{mv_m} \left[ g - \frac{2}{3} \frac{\partial}{\partial w} (wg) \right] - N_0 vgL - N_0 \frac{\partial}{\partial w} (vgM) \quad (28)$$

is the flux in energy space.

#### MAGNITUDE OF SPREAD IN ENERGY LOSS

Like  $L$ ,  $M$  is constructed from individual excitation cross sections. The ratio  $M/L$  is likely much more slowly varying than  $L$  or  $M$  itself, since irregular behavior in the cross sections such as the  $N_2$  resonance spike near 2.5 eV will occur in both  $L$  and  $M$  and divide out in the ratio.

Spread about the mean energy loss  $L$  can be compared with  $L$ . From Eq. (28) it is of order

$$\frac{\text{Diffusive Loss}}{\text{Mean Loss}} \sim \frac{1}{vgL} \frac{\partial}{\partial w} (vgM) \sim \frac{M}{wL} \quad (29)$$

where  $\bar{w}$  is the energy over which  $Mg = (M/L)Lg$  changes much, being of order the swarm temperature or a characteristic energy over which  $L$  itself changes. This ratio is not negligibly small, and can be of order unity, showing that diffusive contributions to energy loss can be comparable to the mean loss, as was the case for energy gain. Since in steady state mean loss essentially balances mean gain, diffusive loss can be as important as diffusive gain in determining the spectrum.

### IMPORTANCE OF ENERGY DIFFUSION

The steady state spectrum from Eqs. (27) and (28) is that for which  $\phi = 0$ , and results from a balance between total energy gain from the electric field and total energy loss to collisions.

It is instructive to temporarily neglect the diffusive contributions to the flux; that is, the  $M$  term in the collision integral, and the term  $-(2/3)\partial(wg)/\partial w$  in the electric field expression. The steady state spectrum one then obtains is that resulting from mean energy gain  $e^2E^2/mv_m$  balanced by mean energy loss  $N_0vL$ . See Figure 1a. This spectrum reduces to a delta function at a single energy  $w_1$  where the rates are equal. Since the mean gain is a decreasing function of  $w$ , while the mean loss is an increasing function, all electrons with  $w > w_1$  lose energy faster than they gain it, and all electrons with  $w < w_1$  gain energy faster than they lose it. All electrons thereby end up with energy  $w_1$ . Thus the physical process which actually determines the energy spectrum is spread in energy gain or loss about the mean. Mean gain and loss rates determine only the average energy in the swarm.

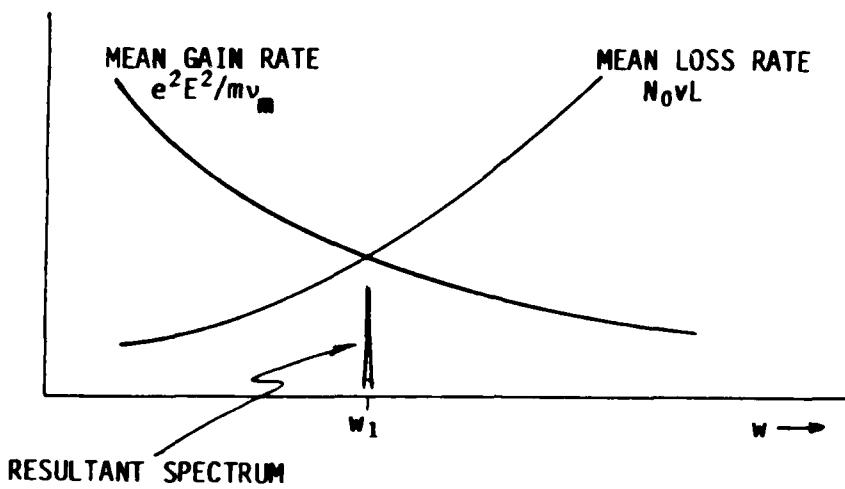


Figure 1a Balance of mean gain and loss rates.  
Resultant spectrum is a  $\delta$  function at  $w_1$ .

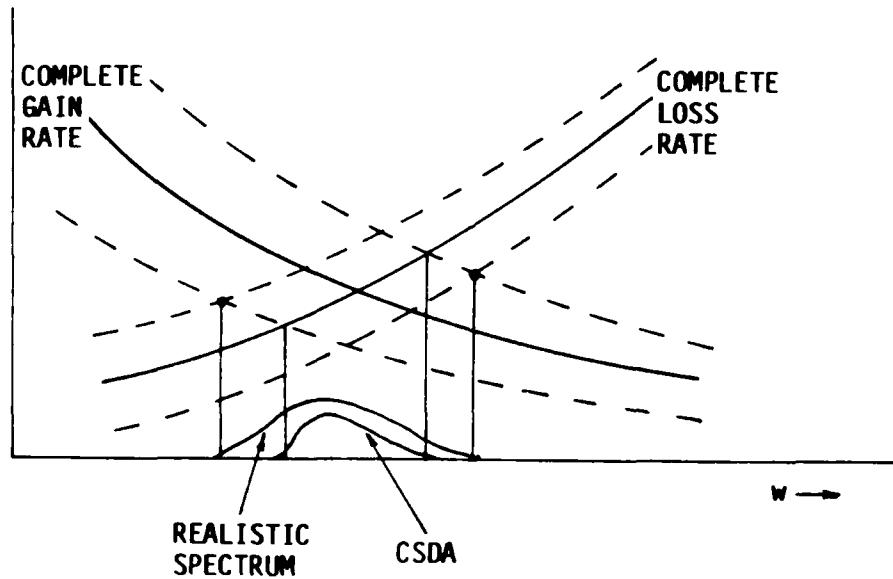


Figure 1b Balance of complete gain and loss rates.  
CSDA neglects spread in energy loss.

It is clear that for electrons with a spread in energies to be in steady state there must be a balance between gain and loss rates over a spread in energies, and this spread determines the spectrum.

This shows that in the CSDA, the only physical process which establishes the spectrum, that is, gives body to the distribution function, is energy diffusion due to elastic scattering in the electric field, since in the collision integral only the mean loss rate is retained. Figure 1b illustrates the CSDA and a realistic spectrum.

Since energy diffusion is so important, we must keep the diffusive contribution in  $C_g$  as well to deduce a realistic spectrum. While L is the lowest order term in the expansion of  $C_g$ , it affects only the average swarm energy. M is the lowest order contributor from the collision integral to the energy distribution.

As Figure 1b shows, the CSDA is poor because it retains energy diffusion in the E-field energy gain term, but neglects it in energy loss processes. That is, it neglects "half" of the physics determining the spectrum.

From this point of view we see that M should not be considered just another term in a Taylor Series expansion of a function. Rather it represents a critical piece of physics that determines the distribution function, and must not be neglected. The functional form in which M appears is a Fokker-Planck approximation to the true random walk. The approximation will be best when the energy loss per collision is small compared with the energy spread in the entire spectrum. Similar to the usual Fokker-Planck equation, it assumes large energy changes occur as a succession of small ones.

The L, M approximation to  $C_g$  is, of course, local in energy space, as is any differential approximation to a random walk problem.

If the energy loss  $w_k$  is extremely small compared with  $w$ , then Equations (23) show  $M \ll wL$ , and the CSDA will be adequate. This happens, for example in elastic collision recoil as mentioned after Eq. (25). If  $w_k$  is comparable with  $w$  or the spectrum spread, then the Fokker-Planck diffusion approximation breaks down. This begins to happen in  $N_2$  at average energies of, say, 1 or 2 eV when energetic tail electrons can excite electronic transitions and  $w_k \sim 7$  eV, or at  $\sim .01$  eV where rotational jumps have comparable energy. There is an interesting intermediate regime where the dominant  $w_k$  is sufficiently smaller than  $w$  but not negligible. This appears to be the case in  $N_2$  for  $E/N_0 \gtrsim .01$  Td, giving the swarm energies greater than rotational jumps, and where vibrational transitions dominate. Even at 1 or 2 eV, electronic transitions induced by the tail are only a part of the energy loss, and the diffusion approximation is still not bad.

One important feature of keeping  $M$  is that this term allows some electrons to lose energy slower than the mean, thereby supporting the high energy tail of the spectrum, as seen graphically in Figure 1b. This will greatly increase the avalanche rate over the CSDA.

We have still neglected third and higher derivatives in the expansion Eq. (22). The main properties of any normalized distribution with a decaying tail, such as  $F$  or  $g \sim \sqrt{w} F$ , are its average energy and the "width" of the function about the average. The first derivative term  $L$  determines the average energy, and the second derivative term  $M$  determines the width, together with corresponding terms from the field contribution. Higher neglected terms could affect only the detailed shape of the function. For example, the third derivative would alter the asymmetry of the spectrum about the mean, and the fourth derivative would set the kurtosis. The transport coefficients of interest are weighted integrals over the spectrum, and the details of the spectrum tend to integrate out. Thus there is physical reason to expect that stopping with  $L$  is insufficient (CSDA) but stopping with  $M$  is sufficient to calculate a spectrum

which reproduces bulk transport coefficients with some acceptable accuracy. These arguments may be less true for the avalanche coefficient at low temperatures which requires an accurate high energy tail.

### CORRECTIONS FOR GAS HEATING

Equations (23) for the inelastic parts of L and M are expressions for the gas at rest. Thermal effects were mentioned only in connection with the elastic part of L in Eq. (12). In fact the Davydov correction for thermal motion of molecules shows that collision calculations are to be modified by replacing g by:

$$g \rightarrow g + T_g \sqrt{w} \frac{\partial}{\partial w} \left( \frac{g}{\sqrt{w}} \right) \quad (30)$$

or, in terms of F(v):

$$F \rightarrow F + T_g \frac{\partial F}{\partial w} \quad (31)$$

Therefore thermal gas motion is taken into account by replacing the flux  $\phi$  in Eq. (28) by

$$\begin{aligned} \phi = & \frac{e^2 E^2}{m v_m} [g - \frac{2}{3} \frac{\partial}{\partial w} (wg)] - N_0 v L [g + T_g \sqrt{w} \frac{\partial}{\partial w} \left( \frac{g}{\sqrt{w}} \right)] \\ & - \frac{\partial}{\partial w} \{N_0 v M [g + T_g \sqrt{w} \frac{\partial}{\partial w} \left( \frac{g}{\sqrt{w}} \right)]\} \end{aligned} \quad (32)$$

The steady state spectrum is that for which  $\phi = 0$ . When  $E \rightarrow 0$  as well, the solution of (32) clearly reduces to a Maxwellian, as it must, for then  $g + T_g \sqrt{w} d(g/\sqrt{w})/dw = 0$ .

## SECTION 4

### EQUATION FOR TIME DEPENDENCE OF ENERGY SPECTRUM

Dropping the Davydov terms, equations (27) and (28) (or (32) with  $T_g = 0$ ) control the time evolution of the energy spectrum in the absence of sources and sinks:

$$\frac{\partial q}{\partial t} + \frac{3}{\partial w} \left\{ \frac{e^2 E^2}{m v_m} [q - \frac{2}{3} \frac{\partial(wq)}{\partial w}] - N_0 v L g - N_0 \frac{\partial(v g M)}{\partial w} \right\} = 0 \quad (33)$$

Sources and sinks are to be added to the right hand side for a specific problem as appropriate. Eq. (33) is valid for  $E$  varying slowly compared with the momentum transfer frequency  $v_m$ , but on any time scale relative to the mean energy transfer frequency. Since  $v_m > 10^{11}/sec$  in sea level air, Eq. (33) will apply to many problems of interest. For example, following a pulsed ionization source, for which the starting spectrum is the initial condition to Eq. (33), this equation determines the relaxation of the spectrum toward equilibrium in the electric field and warm gas.

For situations where  $E = 0$ , the resulting equation

$$\frac{\partial q}{\partial t} - N_0 \frac{\partial}{\partial w} [v L g + \frac{\partial(v g M)}{\partial w}] = 0 \quad (34)$$

determines the relaxation of  $q$  from an initial condition toward thermal equilibrium. Without the  $E$  term, Eq. (34) is no longer limited by  $v_{drift} \ll v_{thermal}$  (two term Legendre series), and so applies to electrons of any energy. It includes mean energy loss, straggling, and thermal heating (through thermally populated rotational states in  $L$  and  $M$ ).

If straggling were to be neglected (CSDA), the resulting equation

$$\frac{\partial g}{\partial t} - N_0 \frac{\partial}{\partial w} (vgL) = 0 \quad (35)$$

would show simple convection in energy space, and laminar flow. That is, electrons of higher energy would never overtake ones of lower energy. Straggling destroys laminar flow, and permits passing in energy space, as actually occurs in a random walk, and spreads out the spectrum.

## SECTION 5 STEADY STATE SPECTRUM

In steady state, the solution for  $F = (m/v)g$  of Eq. (33) with  $\partial g / \partial t = 0$  is

$$F = F_0 \exp \left\{ - \int_{-\infty}^w \frac{L + \frac{1}{w} \frac{\partial}{\partial w} (wM)}{\frac{(eE/N_0)^2}{3 \sigma_m} + M} dw \right\} \quad (36)$$

where  $F_0$  is a normalization constant set by Eq. (4). This spectrum is an improvement over the CSDA

$$F = F_0 \exp \left\{ - \int \frac{3 \sigma_m L}{(eE/N_0)^2} dw \right\} \quad (37)$$

which results when  $M$  is neglected. Both have a quite simple functional form.

### THE DRUYVESTEYN SPECTRUM

The Druyvesteyn spectrum is recovered from Eq. (37) in the special case of  $\sigma_m = \text{constant}$  and elastic collisions only,

$$L = L_{el} = \frac{2m}{M_0} \sigma_m w . \quad (38)$$

Then,  $F$  reduces to

$$F = F_0 \exp\left\{-\frac{3m \sigma_m^2 w^2}{M_0(eE/N_0)^2}\right\} \quad (39)$$

In this same special case the more correct Eq. (36) is essentially the same as (39) because, for elastic collisions only,  $M \sim (2m/M_0)wL \ll wL$ , and the  $M$  correction is negligible. Thus the improved spectrum does not mar already good agreement with data.

It is when inelastic collisions are important that the difference between (36) and (37) is significant.

#### THE NEW TERMS

In Section 6 it will be shown that the two terms  $(eE/N_0)^2/3 \sigma_m$  and  $M$  in the denominator of Eq. (36) can be identified as diffusion coefficients in energy space due to elastic scattering in the electric field (first term) and due to spread in energy loss about the mean ( $M$  term). The total diffusion coefficient is just the sum of the two.

The first term  $L$  in the numerator is the mean rate of energy loss (or gain, if  $L$  is negative) due to collisions. The second term  $(1/w)d(wM)/dw$  is a mean loss (or gain) rate due to energy variation of the diffusion coefficient  $M$ .

At energies below vibrational excitation, and neglecting elastic scattering, only rotational states contribute to  $L$  and  $M$ . We shall use the Gerjuoy-Stein rotational cross sections to evaluate this contribution (Appendix A). States  $\Delta J = 2$  apart are spaced by  $(4J-2)B_0$ , where  $B_0$  is the rotational constant. The cross section for de-excitation,  $\sigma_{J,J-2}$  diverges as  $\sqrt{4JB_0/w}$  when  $w \lesssim 4JB_0$ . In nitrogen,  $B_0 = 2.5 \times 10^{-4}$  eV. This

causes a formal divergence in the numerator term  $(1/w)d(wM)/dw$ , and effectively makes the spectrum unreliable for  $w \gtrsim 10^{-3}$  eV, and the calculated transport coefficients inaccurate for  $E/N_J \gtrsim 10^{-2} T_d$ . When  $w \gtrsim 4JB_J$  diffusion is no longer a good approximation. For numerical calculations we have simply smoothed out the divergence by multiplying this numerator term by  $w/(w+8J)$ . The inaccuracies in characteristic energy and drift velocity will be seen in Section 7.

### THE LOW ENERGY THERMAL LIMIT

For vanishingly small electric fields, the remaining terms in Eq. (36) should make  $F$  reduce to a Maxwellian at  $T_g$ . Thus we should have

$$\frac{L + w^{-1} \partial(wM)/\partial w}{M} = \frac{1}{T_g} \quad (40)$$

or, solving for  $M$ ,

$$M = \frac{1}{w} \int_w^\infty e^{-(w'-w)/T_g} w' L(w') dw' \quad (41)$$

$M$  must be a weighted integral of  $L$  over an energy span about  $T_g$ .

Since  $T_g$  enters  $L$  and  $M$  only through rotational populations (we neglect vibrational temperature), Eq. (40) should hold if we consider only the rotational contributions. Upon constructing  $L$  and  $M$  (Appendix A) one finds Eq. (40) is in general not true. Rotational levels with  $J = 10$  or larger exist, and so energy jumps  $4JB_J = 4 \times 10 \times 2.5 \times 10^{-4} = .01$  eV in  $N_2$  occur, encroaching on electron thermal energies  $\sim .02$  eV. That is, the diffusion approximation breaks down at these low energies, and Eq. (36) is not a good approximation to the spectrum.

However in a hypothetical gas with  $B_0 \rightarrow 0$ , all energy jumps are small, and Eq. (36) is correct. For such a gas, Eq. (40) should hold. In Appendix A, using the Gerjuoy-Stein rotational cross sections, we take the limiting expressions of L and M for  $B_0 \rightarrow 0$ , and show explicitly that Equations (40) and (41) are indeed true, independent of all cross section parameters. According to equilibrium statistical mechanics, this "must" happen, but it is comforting to see it follow from a direct calculation using actual cross sections.

Using the complete L and M for  $N_2$ , the actual spectrum of Eq. (36) with  $E = 0$  is shown in Figure 2. Above about .01 eV it is indeed Maxwellian at the correct temperature, 300 K. (The departure in the high energy tail above 0.3 eV is because we assume the gas is in the vibrational ground state). But near .01 eV there is a non-Maxwellian dip due to "large" energy jumps not well modelled by the Fokker-Planck form. This irregular behavior goes away as  $B_0 \rightarrow 0$ .

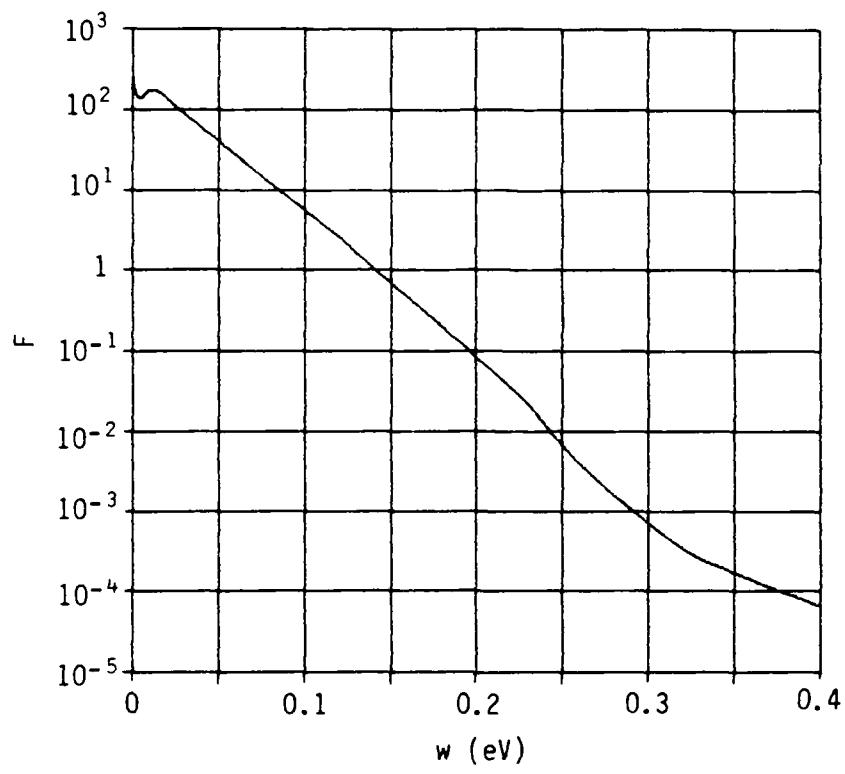


Figure 2. Spectrum in  $N_2$  from Equation (36) when  $E=0$ . Dip near .01 eV is due to rotational transitions of comparable energy. Gas at 300K.

## SECTION 6

### RELATION TO ORDINARY DIFFUSION THEORY

The functional form, Eq. (36), for  $F$  has a simple interpretation in terms of elementary diffusion and convection theory.

Let a quantity  $\psi$  diffuse and convect in one dimension  $x$  with diffusion coefficient  $D$  and convection velocity  $V$ :

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x} (V\psi) = \frac{\partial}{\partial x} D \frac{\partial \psi}{\partial x} . \quad (42)$$

We shall presently identify  $x$  with  $w$  and  $\psi$  with  $g$ .  $V$  and  $D$  may be functions of  $x$ . In steady state, the elementary diffusion-convection equation (42) shows that the flux must be constant in  $t$  and  $x$ :

$$V\psi - D \frac{\partial \psi}{\partial x} = \text{constant} = 0 . \quad (43)$$

We assume  $\psi$  and its derivative vanish at some end point, so the constant is taken to be zero. Then

$$\frac{1}{\psi} \frac{\partial \psi}{\partial x} = \frac{V}{D} . \quad (44)$$

In steady state the (prescribed) convection velocity and diffusion coefficient determine the logarithmic derivative of the dependent variable by Equation (44). Consequently  $\psi$  is distributed according to

$$\psi(x) = \psi_0 e^{\int \frac{V}{D} dx}, \quad (45)$$

where  $\psi_0$  is a normalization constant.

If we now take  $x$  to be the electron energy  $w$ , and  $\psi$  the spectrum  $g$ , the controlling equation Equation (33)

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial w} \left[ \frac{e^2 E^2}{mv_m} \left( g - \frac{2}{3} \frac{\partial}{\partial w} (wg) \right) \right] - N_0 v L g - \frac{\partial}{\partial w} (N_0 v M g) = 0 \quad (46)$$

can be put in the canonical form of Equation (42) by expanding derivatives and defining

$$D_i = N_0 v M \quad (47)$$

as the coefficient of diffusion due to straggling from inelastic energy loss collisions,

$$D_E = \frac{2}{3} w \frac{e^2 E^2}{mv_m} \quad (48)$$

as the coefficient of diffusion due to momentum transfer scatterings in the electric field, and the following convection velocities:

$$v_1^E = \frac{e^2 E^2}{mv_m} = \text{mean energy gain rate in electric field} \quad (49)$$

$$v_2^E = - \frac{2}{3} \frac{e^2 E^2}{mv_m} = \text{gain (or loss) rate arising from energy dependence of } D_E \quad (50)$$

$$v_1^i = - N_0 v L = \text{mean loss rate due to inelastic collisions} \quad (51)$$

$$v_2^i = - \frac{\partial}{\partial w} (N_0 v M) = \text{energy drift due to } \frac{\partial D_i}{\partial w} . \quad (52)$$

Diffusion coefficients have dimensions energy<sup>2</sup>/time, and velocities have dimensions of energy/time. The energy dependence of  $D_E$  and  $D_i$  cause a mean flux ( $v_1^E$  and  $v_2^i$ ) because of the way they appear in Eq. (46) under the  $\nabla^2/\partial w^2$  operator. Eq. (46) can then be written

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial w} (Vg) = \frac{\partial}{\partial w} (D \frac{\partial g}{\partial w}) \quad (53)$$

with

$$\begin{aligned} V &= v_1^E + v_2^E + v_1^i + v_2^i \\ &= N_0 v \left[ \frac{(eE/N_0)^2}{3mv^2\sigma_m} - L - \frac{1}{v} \frac{\partial}{\partial w} (vM) \right] \end{aligned} \quad (54)$$

and

$$\begin{aligned} D &= D_E + D_i \\ &= N_0 v \left[ \frac{(eE/N_0)^2}{3\sigma_m} + M \right] . \end{aligned} \quad (55)$$

Following Eq. (45) the steady state solution of Eq. (53) is

$$g = g_0 \exp \left( \int \frac{V}{D} dw \right) . \quad (56)$$

Forming the ratio  $V/D$  from Equations (54) and (55), we add and subtract  $M/2w$  in the numerator, and use  $v^{-1}(\partial/\partial w)(vM) + M/2w = w^{-1}(\partial/\partial w)(wM)$  to find

$$\frac{V}{D} = \frac{1}{2w} - \frac{\frac{L}{w} + \frac{1}{w} \frac{\partial}{\partial w} (wM)}{\frac{E'^2}{3\sigma_m} + M} , \quad (57)$$

where  $E' = eE/N_0$  is the reduced electric field. Upon integrating and exponentiating, the first term ( $1/2w$ ) becomes  $\sqrt{w}$ , and the remaining factor is therefore  $F$ ,

$$F = F_0 \exp \left\{ - \int_0^w \frac{\frac{L}{w} + w^{-1} \frac{\partial(wM)}{\partial w} dw}{E'^2/3\sigma_m + M} \right\} \quad (58)$$

as in Eq. (36). Thus the functional form for the steady state energy spectrum is an elementary consequence of ordinary convection and diffusion in energy space, as is the time dependent equation (46) or (33).

This can be seen as well by writing the flux, Eq. (28), in terms of  $F$ . After some algebra it becomes

$$\phi = - \frac{2wN_0}{m^2} \left\{ \left[ L + \frac{1}{w} \frac{\partial(wM)}{\partial w} \right] F + \left[ \frac{E'^2}{3\sigma_m} + M \right] \frac{\partial F}{\partial w} \right\} , \quad (59)$$

the coefficients of  $F$  and  $\partial F/\partial w$  being the convection velocity numerator and diffusion coefficient denominator, respectively, of the integral in Eq. (58).

## SECTION 7 THE CASE OF NITROGEN

We apply these ideas to  $N_2$ .  $L$  and  $M$  are constructed from cross section data. The steady state spectrum, Eq. (36), and swarm parameters are then computed.

### CROSS SECTIONS, AND L AND M FUNCTIONS

Electron-molecule cross sections are compiled in a number of places (refs 9 - 12). Reference 13 is a recent critique of rotational and vibrational excitations. Here we use the Gerjuoy-Stein expressions (ref 14) for rotational cross sections, with the  $N_2$  quadrupole moment  $Q = 1.04$  in units of  $ea_0^2$ .

For the vibrational and electronic cross sections, we use a set compiled by Archer (ref 15) that has been in use in the DNA Auroral physics community for years. These vibrational excitations are based on the measurements by Schulz as normalized by Haas. A low energy (0.29 - 1.7 eV) tail for the  $v = 0 - 1$  transition was added as suggested by Englehardt, Phelps, and Risk (Ref. 6). Numerical values for the tail were taken from the second table on page 64 of Kieffer (Ref. 16). The electronic cross sections agree quite well with those tabulated by Wadzinski and Jasperse (ref 11).

$L$  and  $M$  for  $10^{-3} < w < 10^2$  eV are shown in Figure 3a.  $L$  becomes negative for  $w < T_g \sim .025$  eV, because a lower energy electron gains

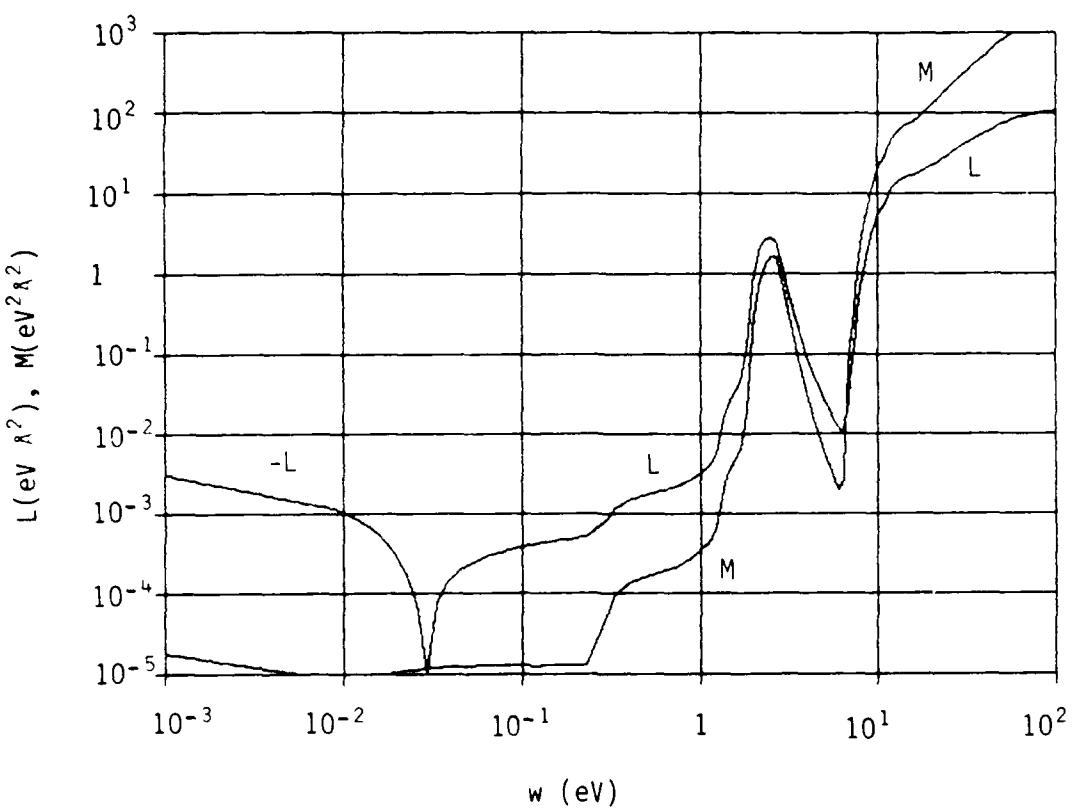


Figure 3a.  $M$  and  $L$  functions for  $N_2$  at 300 K.

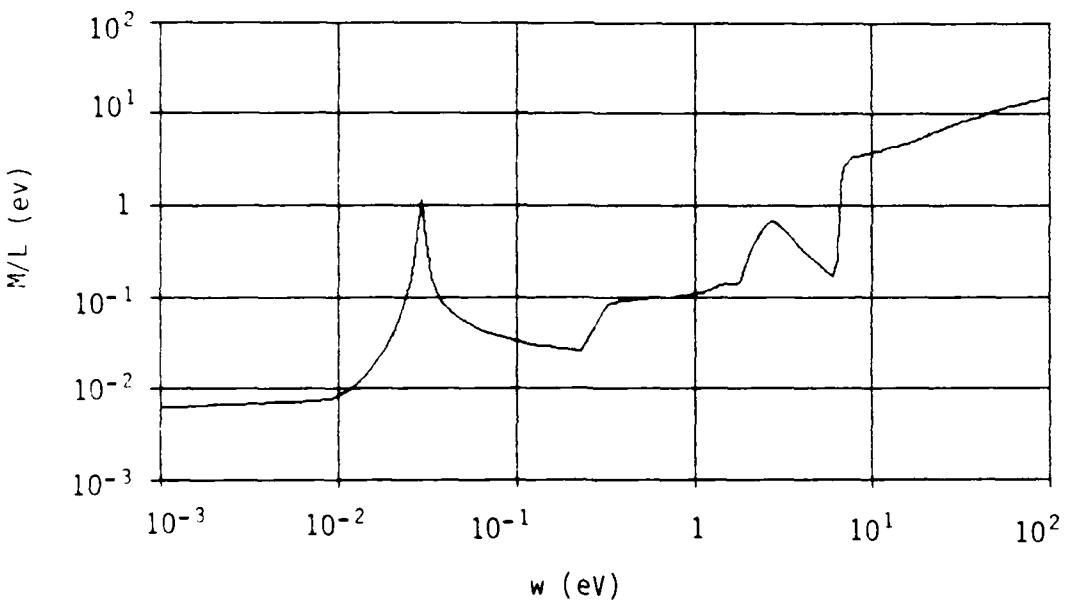


Figure 3b.  $M/L$  for  $N_2$  at 300 K.

energy on the average by collisions with the gas at this temperature from super-elastic rotational transitions.  $M$ , of course, is always positive. Over  $10^{-3}$  to 10 eV, these functions vary by more than six orders of magnitude. The ratio  $M/L$  is shown in Figure 3b. It is much more slowly varying than  $M$  or  $L$  itself.

### THE ENERGY SPECTRUM

Figures 4 and 5 show the energy spectrum  $F$ , Eq(36), for  $E/N_0 = 10 \text{ Td}$  and  $100 \text{ Td}$ , respectively.  $1 \text{ Td} = 10^{-17} \text{ V-cm}^2$ . The high energy tail is markedly higher than in the CSDA which is also shown. Any process with significant cross section above the CSDA tail will have markedly different rates with the two spectra.

Figure 5 also shows a spectrum from the calculation by Pitchford and Phelps (Ref. 17), involving a numerical solution of the Boltzmann Equation with complete collision integral. These authors used a different cross section set, so the comparison is not meaningful in a precise sense. Nevertheless the differences are noteworthy. In particular, we overestimate the high energy tail and underestimate the low energy population below 2 eV. This is due to the local diffusion approximation. Electronic transitions allow high energy electrons to jump to very low energies more quickly than in the diffusion model. This excessive tail will also cause a large avalanche coefficient discussed later.

Eq. (36) also shows a curious broad plateau around 3.5 to 7 eV, absent in the more complete calculation. This too is likely due to electronic transitions which permit electrons to jump over this energy range. In general it is clear the average swarm energy at 100 Td will be computed to be too large.

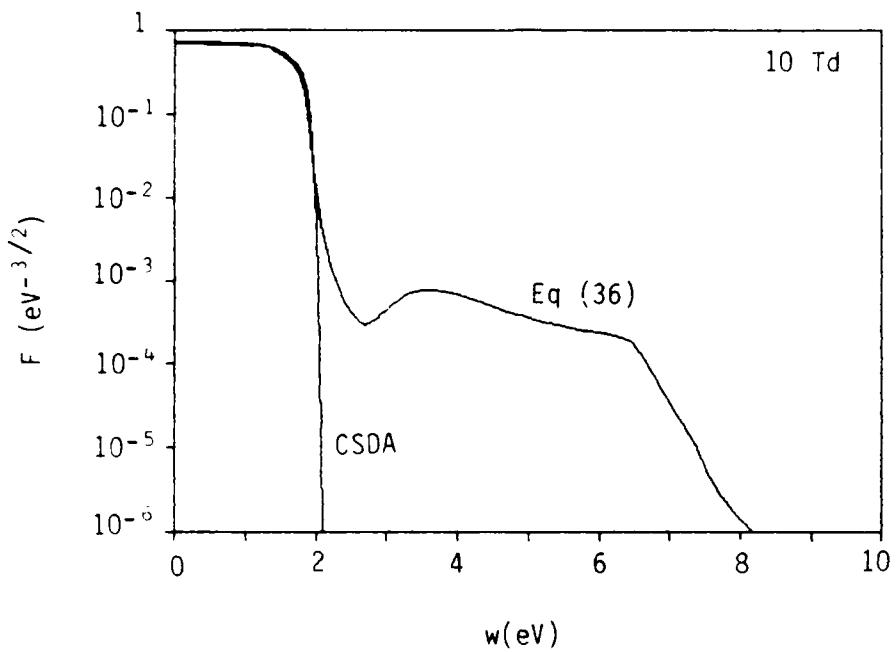


Figure 4. Energy spectrum at  $E/N_0 = 10^{-16} \text{ V-cm}^2$  from Eq. (36) and in the CSDA.

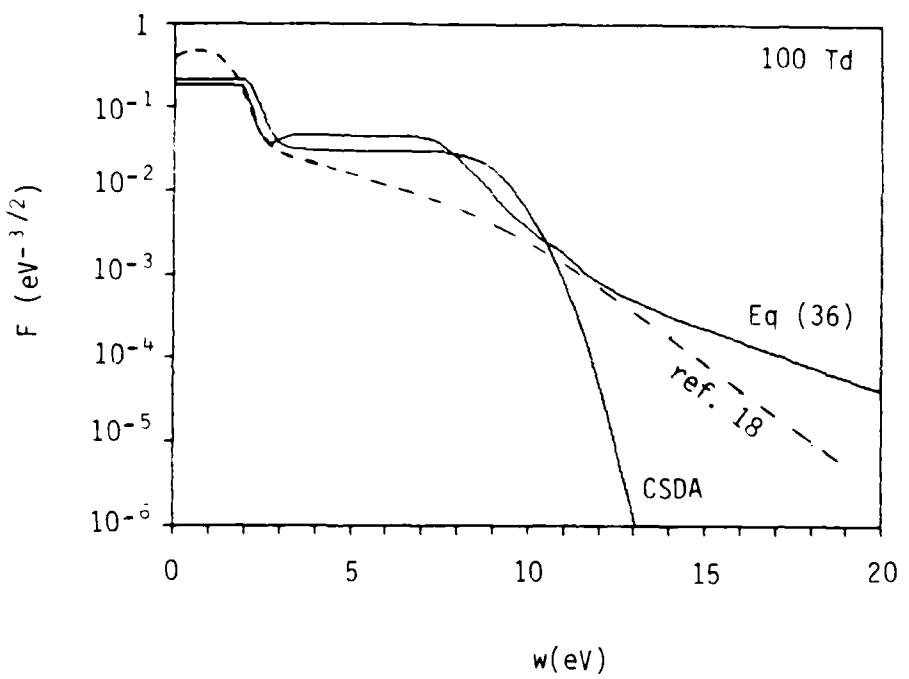


Figure 5. Energy spectrum at  $10^{-15}$  V-cm $^2$  from Eq. (36), the CSDA, and Reference 18.

## TRANSPORT COEFFICIENTS

The open circles in Figure 6 show the drift velocity calculated with Eq(36) superimposed on data compiled by Dutton (ref 8). It is slightly too small below, say,  $3 \times 10^{-19}$  V-cm<sup>2</sup>. Here the Fokker-Planck approximation is in jeopardy because rotational transitions become comparable to swarm energies. Refer to the spectrum in Figure 2 at zero field. Average energies are slightly too large as seen momentarily.

The drift velocity is also too small near  $10^{-16}$  or  $10^{-15}$  V-cm<sup>2</sup>. Here the spectrum is similar to that in Figure 5, and average energies are again too high.

At stronger fields the drift velocity returns to good agreement. But at these larger energies the mono-energetic momentum transfer collision frequency in N<sub>2</sub>,  $N_0 v \sigma_m$ , is slowly varying with energy, and the drift velocity is only weakly dependent on the spectrum.

At fields less than 0.1 Td, we find drift velocities computed in the CSDA to be more than 20% too small, and characteristic energies more than 30% too large. But in stronger fields, we find CSDA drift velocities to be more like 5 to 12% too small, and characteristic energies 5 to 13% larger than in the diffusion approximation.

The swarm characteristic energy is shown in Figure 7. It is slightly too large below about  $3 \times 10^{-19}$  V-cm<sup>2</sup>, and is significantly too large above  $10^{-15}$  V-cm<sup>2</sup>, accounting for the lowered drift velocities. As mentioned, this is due to finite rotational and electronic energy jumps in these two regions.

The swarm momentum transfer ( $\bar{v}_m$ ) and energy transfer ( $v_u$ ) collision frequencies are shown in Figure 8, superimposed on a graph from Frost

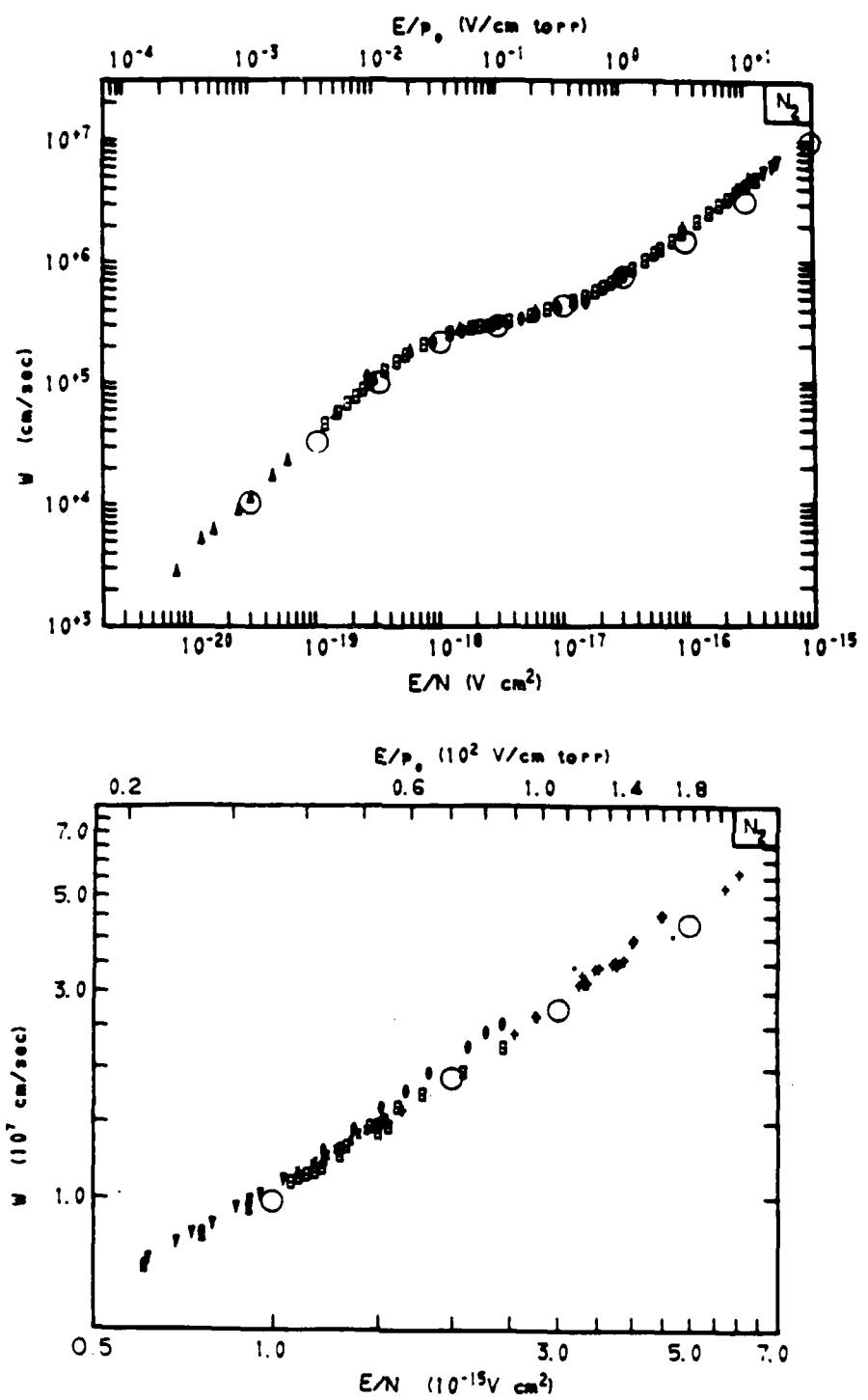


Figure 6. Calculated  $N_2$  drift velocity (open circles) with data compiled by Dutton (Ref. 8).

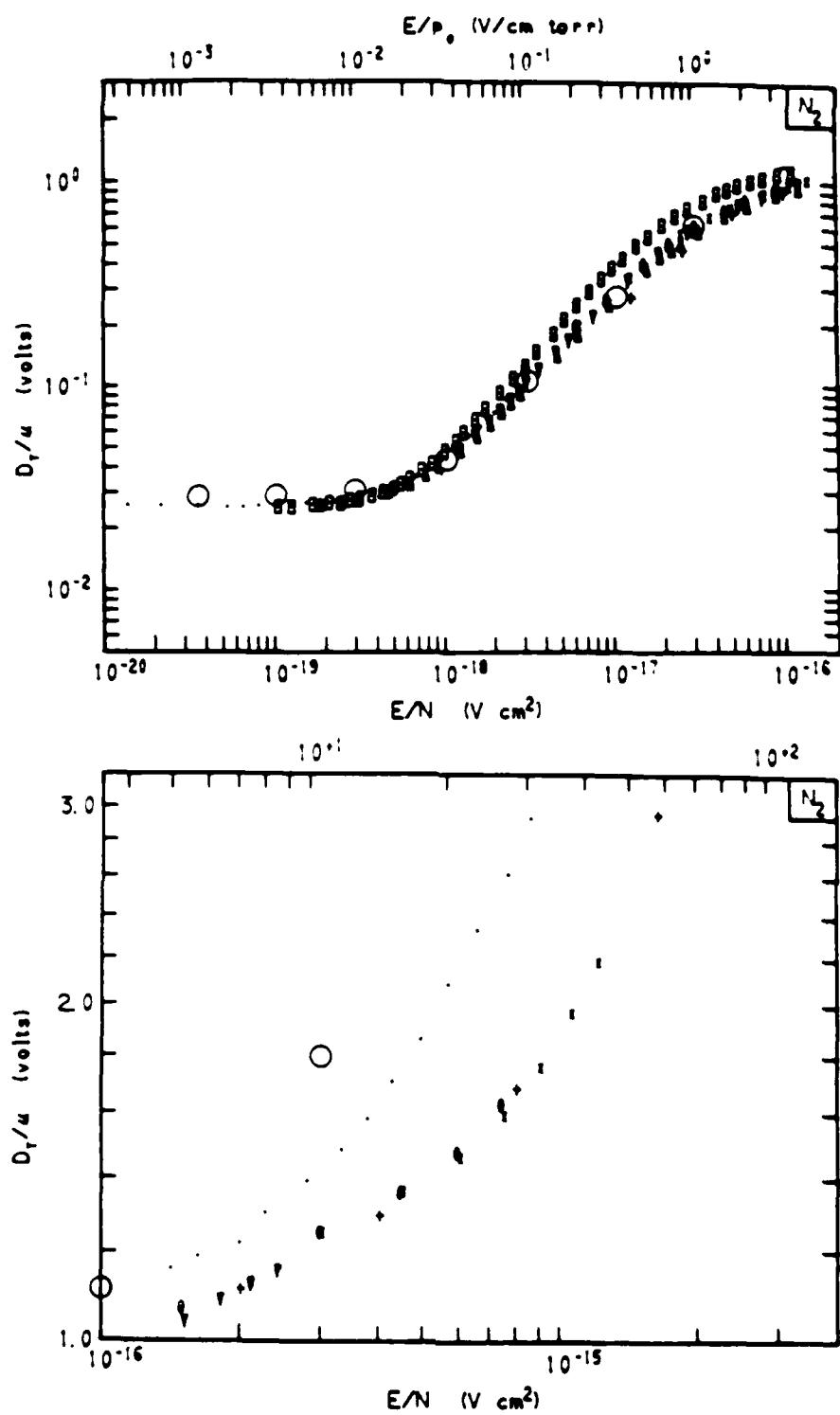


Figure 7. Calculated swarm characteristic energies in  $N_2$  (open circles) with data compiled by Dutton (Ref. 8). Ambient temperature (300 K).

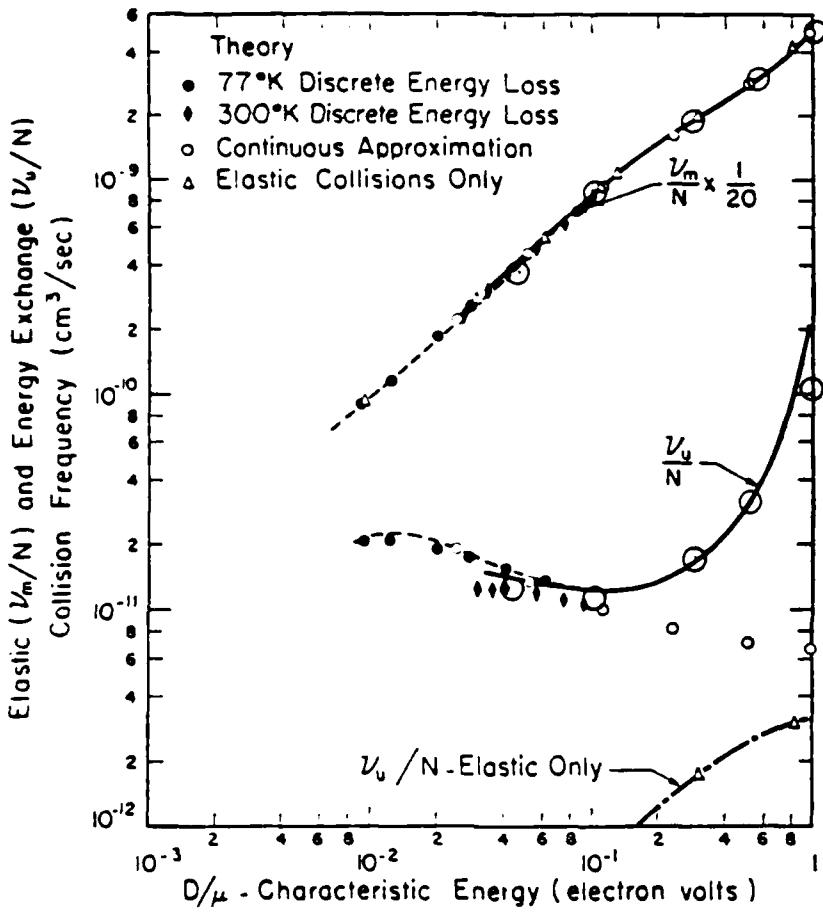


Figure 8. Swarm momentum transfer ( $v_m/N$ ) and energy transfer ( $v_u/N$ ) collision frequencies. The large open circles are our calculated values, superimposed on a graph from Frost and Phelps (Ref. 18). The solid curves are averaged experimental data at 300 K. The other four sets of points are various theories within Ref. 18.

and Phelps (Ref. 18). They are defined by

$$\bar{v}_m = \frac{eE}{mv_{\text{drift}}} \quad (60)$$

$$v_u = \frac{eE v_{\text{drift}}}{D/\mu - T_g} \quad (61)$$

where  $\mu$  is the mobility, and  $D/\mu$  is the swarm characteristic energy. (Ref. 18 uses  $v_m$  for the swarm frequency, a symbol we have reserved for the mono-energetic collision frequency.) The agreement is striking except for  $v_u$  near 1 eV. The dependence of  $v_u$  on  $v_{\text{drift}}$  and  $D/\mu$  accentuates the dependence on the swarm average energy.

The non-self-consistent avalanche coefficient,  $\alpha(\text{cm}^{-1})$ , was computed by

$$\alpha = \frac{1}{v_{\text{drift}}} \int dw g v \sigma_i \quad (62)$$

where  $\sigma_i$  is the total  $N_2$  ionization cross section. It is shown as open circles in Figure 9, superimposed on data of Dutton. Below about 300 Td the CSDA, shown as crosses, is, of course, woefully low. Eq. (36) is too high by more than an order of magnitude at 100 Td, a disconcerting amount. The spectral tail seen in Figure 5 is responsible.

## DISCUSSION

With some exceptions (avalanche rate, characteristic energy when near several eV) the Fokker-Planck approximation to the energy spectrum

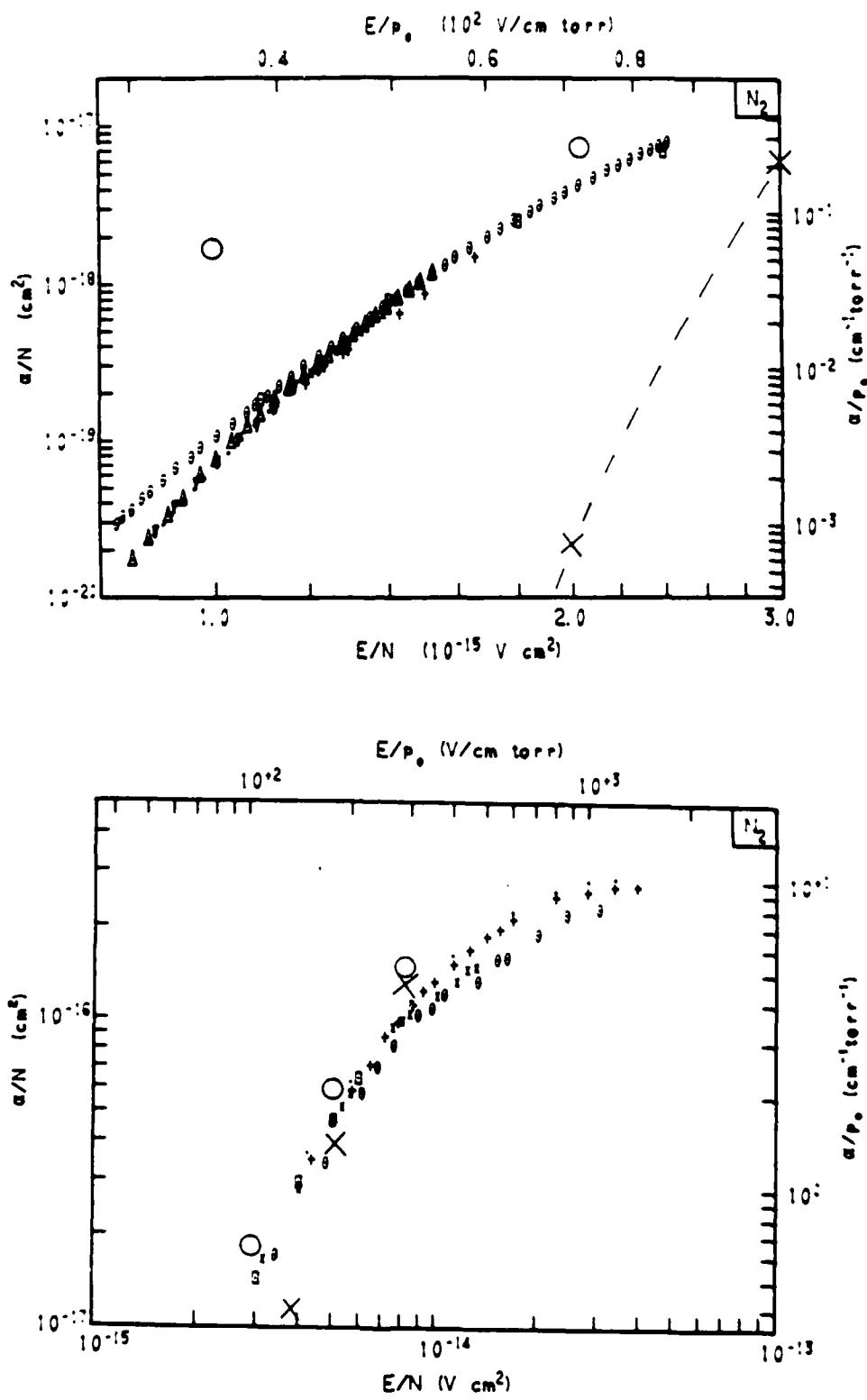


Figure 9. Calculated avalanche rates (open circles) with data compiled by Dutton (Ref. 8). Crosses (x) are CSDA calculations.

appears to be able to reproduce transport coefficients in  $N_2$  with reasonable accuracy. Other gases are under study. Inaccuracies show up when molecular energy jumps are not small compared with swarm energies, precisely when the diffusion approximation becomes unreliable. These features are understandable when it is realized that it is the spread of energy gain and loss about the mean rates that actually determine the spectrum.

At present the ultimate utility of the diffusion approximation is unclear. It depends in part on the success in other gases. It may be quite useful for rough calculations, it being possible to obtain spectra and all transport coefficients merely by numerical quadratures. The time dependent equation (33) may be especially useful, being a significant improvement over the CSDA, but not substantially more complicated.

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APPENDIX A  
ROTATIONAL CONTRIBUTION TO L AND M

The rotational contribution to  $C_g^{\text{inel}}$ , Eq. (21), is

$$C_{\text{rot}} = \sum_{J=0}^{\infty} N_J [ (g\sigma_{J,J+2})_{w+w_{J,J+2}} - (g\sigma_{J,J+2})_w ] + \sum_{J=2}^{\infty} N_J [ (g\sigma_{J,J-2})_{w-w_{J,J-2}} - (g\sigma_{J,J-2})_w ] \quad (\text{A-1})$$

since only  $J \pm 2$  are accessible from  $J$  for a quadrupole interaction. The second line in Eq. (A-1) is collisions of the second kind, in which an electron gains energy.  $N_J$  is the number of molecules in the  $J$ -th state,

$$N_J = N_0 \frac{P_J \exp(-E_J/T_g)}{\sum P_J \exp(-E_J/T_g)} , \quad (\text{A-2})$$

$$P_J = 3(1+a)(2J+1) , \quad (\text{A-3})$$

$$E_J = J(J+1)B_0 ,$$

and  $a=0$  for odd  $J$ ,  $a=1$  for even  $J$ . The transition energies are

$$W_{J,J+2} = E_{J+2} - E_J = (4J+6)B_0 \quad (\text{A-4})$$

$$W_{J,J-2} = E_J - E_{J-2} = (4J-2)B_0$$

The cross sections for excitation and de-excitation are taken as those of Gerjuoy and Stein (Ref. 14).

$$\sigma_{J,J+2} = \frac{(J+2)(J+1)}{(2J+3)(2J+1)} \sigma_0 [1 - \frac{(4J+6)B_0}{w}]^{1/2} \quad (A-5)$$

$$\sigma_{J,J-2} = \frac{J(J-1)}{(2J-1)(2J+1)} \sigma_0 [1 + \frac{(4J-2)B_0}{w}]^{1/2} \quad (A-6)$$

where

$$\sigma_0 = 8\pi Q^2 a_0^2 / 15 \quad (A-7)$$

$$a_0 = \text{Bohr radius} = .529 \times 10^{-8} \text{ cm}$$

and  $Q$  is the molecule quadrupole moment in units of  $ea_0^2$ .  $Q \approx 1.04$  for  $N_2$ .  $B_0$  is the rotational constant,  $= 2.5 \times 10^{-4}$  eV in  $N_2$ .

The expressions for  $L$  and  $M$ , Equations (23) are

$$L_{\text{rot}} = \sum_0^{\infty} N_J w_{J,J+2} \sigma_{J,J+2} - \sum_2^{\infty} N_J w_{J,J-2} \sigma_{J,J-2} \quad (A-8)$$

$$M_{\text{rot}} = \frac{1}{2} \sum_0^{\infty} N_J w_{J,J+2}^2 \sigma_{J,J+2} + \frac{1}{2} \sum_2^{\infty} N_J w_{J,J-2}^2 \sigma_{J,J-2} \quad (A-9)$$

At  $300^\circ$  it takes 20 or 30 terms for the sums to converge (by which point  $E_J/T_g = J(J+1)B_0/T_g \gtrsim 5$ ).

Below the threshold for exciting the lowest state,  $J=0$  to  $J=2$ ,  $w < 6B_0$ ,  $L$  is obviously negative. The electron can only gain energy. All terms together actually make  $L_{\text{rot}}$  negative for  $w < T_g$ .

## THE SMALL $B_0$ LIMIT

We now obtain the limiting expressions for  $L_{\text{rot}}$  and  $M_{\text{rot}}$  when  $B_0 \ll T_g$ , and  $B_0 \ll w$ . Let

$$\alpha = \frac{B_0}{T_g} \ll 1, \quad \gamma = \frac{B_0}{w} \ll 1. \quad (\text{A-10})$$

Inserting the variables in Eq. (A-8) and cancelling common factors in the numerator and denominator we have

$$L = 2A\sigma_0 B_0 \sum_0^{\infty} (1+a)e^{-J(J+1)\alpha} (J+2)(J+1)\sqrt{1-(4J+6)\gamma}$$

$$- 2A\sigma_0 B_0 \sum_2^{\infty} (1+a)e^{-J(J+1)\alpha} J(J-1)\sqrt{1+(4J-2)\gamma} \quad (\text{A-11})$$

where  $A = 3N_0 / \sum_J P_J \exp(-J(J+1)\alpha)$  is a normalization constant.

Many terms, up to  $J \sim \sqrt{5/\alpha}$ , will contribute. Take the average value of  $(1+a)$  to be  $3/2$ , and keep first order in  $\gamma$ :

$$L = 3A\sigma_0 B_0 \sum_0^{\infty} (J+2)(J+1)e^{-J(J+1)\alpha} [1-(2J+3)\gamma]$$

$$- 3A\sigma_0 B_0 \sum_2^{\infty} J(J-1) e^{-J(J+1)\alpha} [1+(2J-1)\gamma] \quad (\text{A-12})$$

The sums will behave as inverse powers of  $\alpha$ , so in the first sum the  $J=0$  and  $J=1$  terms are negligible compared with the remaining  $\sum_2^{\infty}$ . Combining the two remaining sums  $\sum_2^{\infty}$ ,

$$\begin{aligned} \frac{L}{3A\sigma_0 B_0} &= \sum_{J=2}^{\infty} e^{-J(J+1)\alpha} [ (J+2)(J+1) - J(J-1) \\ &\quad - [(J+2)(J+1)(2J+3) + J(J-1)(2J-1)] \gamma ] \quad (A-13) \\ &= 2 \sum_{J=2}^{\infty} e^{-J(J+1)\alpha} [ 2J+1 - [2J^3+3J^2+7J+3] \gamma ] \end{aligned}$$

Higher powers of  $J$  lead to higher powers of  $\alpha^{-1/2}$  in the sums. Keeping leading terms,

$$\frac{L}{3A\sigma_0 B_0} = 4 \sum_{J=2}^{\infty} e^{-J(J+1)\alpha} [ J - J^3 \gamma ] . \quad (A-14)$$

The sums can be approximated by integrals

$$\sum_{J=2}^{\infty} J e^{-J(J+1)\alpha} \approx \int_2^{\infty} x e^{-\alpha x^2} dx \approx \int_0^{\infty} x e^{-\alpha x^2} dx = \frac{1}{2\alpha} \quad (A-15a)$$

$$\sum_{J=2}^{\infty} J^3 e^{-J(J+1)\alpha} \approx \int_0^{\infty} x^3 e^{-\alpha x^2} dx = \frac{1}{2\alpha^2} \quad (A-15b)$$

Then

$$\frac{L}{3A\sigma_0 B_0} = \frac{2}{\alpha} \left( 1 - \frac{\gamma}{\alpha} \right) = \frac{2Tq}{B_0} \left( 1 - \frac{Tq}{w} \right) \quad (A-16)$$

The sum in A is

$$\sum_J P_J e^{-J(J+1)\alpha} \approx \frac{9}{2\alpha} ,$$

so

$$A = 3N_0 / \sum_J P_J e^{-J(J+1)\alpha} = \frac{2}{3} \alpha N_0 \quad (A-17)$$

Equations (A-16) and (A-17) then show the limiting form for L as  $B_0 \rightarrow 0$  to be

$$L = 4N_0 \sigma_0 B_0 \left( 1 - \frac{Tq}{w} \right) . \quad (A-18)$$

Electrons with  $w < T_g$  gain energy.

A parallel calculation for M shows

$$M = 4N_0\sigma_0 B_0 T_g . \quad (A-19)$$

Equations (A-18) and (A-19) are explicit expressions for L and M as  $B_0 \rightarrow 0$ . In this same limit the diffusion approximation to the spectrum should be valid.

#### REDUCTION OF SPECTRUM TO MAXWELLIAN

The steady state spectrum Eq. (36) must become Maxwellian when  $E=0$ . This led to the requirement (40) or (41). We now show these requirements are indeed met when  $B_0 \rightarrow 0$  for then energy jumps are small and the diffusion expressions are good.

With M from Eq. (A-19), and L from (A-18), find

$$\frac{1}{w} \frac{\partial}{\partial w} (wM) = \frac{M}{w} \quad (A-20)$$

and

$$L = \frac{M}{T_g} - \frac{M}{w} \quad (A-21)$$

Thus

$$\frac{L + w^{-1} \frac{\partial (wM)}{\partial w}}{M} = \frac{1}{T_g} \quad (A-22)$$

as required. Likewise the integral relationship (41) between L and M is easily shown to hold.

This shows by explicit calculation that for small energy jumps the diffusion approximation reduces correctly.

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